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Liquid Organic Hydrogen Carriers: Thermophysical and Thermochemical Studies of Benzyl- and Dibenzyl-toluene Derivatives

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Abstract

© 2015 American Chemical Society. The heat transfer oils dibenzyltoluene and benzyltoluene are promising materials as a new class of liquid organic hydrogen carrier compounds (LOHC). Thermophysical properties (heat capacity, density, viscosity, and surface tension) of the commercially available thermofluids Marlothem LH (benzyltoluene) and Marlotherm SH (dibenzyltoluene) and their completely hydrogenated derivatives were measured. Thermochemical properties (enthalpies of combustion and enthalpies of vaporization) were derived from experiments. Gas-phase molar enthalpies of formation were derived and validated with group-additivity and high-level quantum chemical calculations. Enthalpies of the hydrogenation/dehydrogenation reactions of the LOHC pairs under study were derived.

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